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METAL-INSULATOR PHASE DIAGRAM FOR THE FULLY DIAGONAL DISORDERED HUBBARD MODEL AT HALF-FILLING

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Abstract. *The electronic properties of strongly correlated systems with binary type of disorder are investigated using the coherent potential approximation. For half-filled system, two transitions from a band insulator via a metallic state to a Mott insulator are found with increasing the correlation strength of only one of the constituents. Our phase diagram is consistent with those obtained by the dynamical mean field theory.*

Keywords: metal-insulator transition; phase diagram; disordered Hubbard model.

Classification numbers: 71.27.+a.

I. INTRODUCTION

In many materials, both the disorder and the correlation effects are present at the same time. The strong correlation effect between electrons has provided us a lot of interesting phenomena, such as high transition temperature superconductivity, metal-insulator transition (MIT), spin-charge-orbital orderings and so on. On the other hand, real materials are always subject to different kinds of disorder, such as vacancies, impurities and non-stoichiometric composition. Therefore, the disorder and the electron correlation effects should be considered together to understand the electronic properties of the system.

A generic model to study the common influence of disorder and correlations is the Hubbard model including diagonal disorder. For this model, the MIT at noninteger filling have been found by Byczuk et al. [1, 2]. They have shown that at a particular density, equal to the disorder concentration x (or $1+x$), the interplay between disorder-induced band splitting and correlation-induced Mott transition gives rise to a new type of MIT. Recently, a very interesting study on MIT in the disordered and correlated system $SrTi_{1-x}Ru_xO_3$ has been performed [3]. To explain this experiment, Lombardo et al. [4] proposed a model Hamiltonian where both Ru and Ti sites are included. Here, besides the difference between local energies of Ru and Ti ($\varepsilon_A \neq \varepsilon_B$), a difference between

local Coulomb repulsion $U_A \neq U_B$ is introduced. This model was solved using the dynamical mean field theory (DMFT) with the non-crossing approximation (NCA) as the impurity solver. The disorder was treated by the coherent potential approximation (CPA). For half-filled systems, various metal-insulator transitions were described by spectral analysis and a phase diagram was obtained.

It should be noted that the NCA is performed at finite temperature, therefore we propose now to consider the phase diagram at zero temperature using the other method. In this paper we employ the CPA to handle both disorder and correlations in the fully diagonal disordered Hubbard model. Our results support the main results obtained in Ref. [4] and show the simple way to study disordered transition metal oxides where the strong correlated $3d$ orbitals hybridize with non-correlated $2d$ orbitals.

II. MODEL AND SOLVING METHOD

We consider the following Hamiltonian with correlations and binary type of disorder

$$H = -t \sum_{<ij>\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}) + \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_i U_i n_{i\uparrow} n_{i\downarrow}, \tag{1}$$

where $c_{i\sigma}(c^{\dagger}_{i\sigma})$ annihilates (creates) an electron with spin σ at site i, $n_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ and the sum $< ij >$ is the sum over nearest neighbor sites of a Bethe lattice. A fraction x of sites (sites A) have a local on-site energy $\varepsilon_i = \varepsilon_A$ and a local on-site Coulomb repulsion $U_i = U_A$ and a fraction $1-x$ of sites (sites B) have a local on-site energy $\varepsilon_i = \varepsilon_B$ and a local on-site Coulomb repulsion $U_i = U_B$. In addition, we define $\Delta = \varepsilon_A - \varepsilon_B$ the energy difference between the two types of sites. This model describes to an $A_x B_{1-x}$ alloy with fully diagonal disorder.

In the alloy-analog approach the many-body Hamiltonian (1) is replaced by a one-particle Hamiltonian of the form

$$\tilde{H} = \sum_{i\sigma} \tilde{\varepsilon}_{i\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} - t \sum_{<ij>\sigma} (c^{\dagger}_{i\sigma} c_{i\sigma} + \text{H.c.}), \tag{2}$$

where the random potential $\tilde{\varepsilon}_{i\sigma}$ takes the values $\tilde{\varepsilon}^{\gamma}(\gamma = \overline{1,4})$ with the probabilities $p^{(\nu)}_{\sigma}$ [5]

$$\tilde{\varepsilon}_{i\sigma} = \begin{cases} \varepsilon_A & = \tilde{\varepsilon}^{(1)}, \quad p^{(1)}_{\sigma} = x(1-n_{A-\sigma}), \\ \varepsilon_A + U_A & = \tilde{\varepsilon}^{(2)}, \quad p^{(2)}_{\sigma} = x n_{A-\sigma}, \\ \varepsilon_B & = \tilde{\varepsilon}^{(3)}, \quad p^{(3)}_{\sigma} = (1-x)(1-n_{B-\sigma}), \\ \varepsilon_B + U_B & = \tilde{\varepsilon}^{(4)}, \quad p^{(4)}_{\sigma} = (1-x) n_B. \end{cases} \tag{3}$$

The mean occupation numbers $n_{A-\sigma}$ and $n_{B-\sigma}$ must be determined self-consistently. Hereafter, we focus on the paramagnetic case, for which $n_{A\sigma} = n_{A-\sigma} = n_A/2, n_{B\sigma} = n_{B-\sigma} = n_B/2$ and all the one-electron quantities become spin-independent. The local coherent Green function corresponding to the Hamiltonian (2) takes the form [6]

$$G(\omega) = \frac{2}{W} \left[\omega - \Sigma(\omega) - \sqrt{(\omega - \Sigma(\omega))^2 - W^2} \right], \tag{4}$$

provided that a semi-elliptic density of states (DOS) is made for non-interacting electrons $\rho_0(z) = \frac{2}{\pi W^2}\sqrt{W^2 - z^2}$ (W is the half-width of the band) and $\Sigma(\omega)$ denotes the coherent potential which is determined self-consistently. The CPA demands that the scattering matrix vanishes on average over all possible disorder configurations.

This is equivalent to

$$G(\omega) = \sum_{\nu=1}^{4} p^{(\nu)} G(\omega)^{(\nu)}, \tag{5}$$

where

$$G^{\nu}(\omega) = \frac{G(\omega)}{1-(\tilde{\varepsilon}^{(\nu)} - \Sigma(\omega))G(\omega)}. \tag{6}$$

For a given mean electron number (per site) n the Fermi energy E_F at zero temperature is determined by

$$n = 2\int_{-\infty}^{E_F} \rho(\omega) d\omega = x n_A + (1-x) n_B, \tag{7}$$

where

$$n_A = 2\int_{-\infty}^{E_F} d\omega \left[(1-n_A/2)\rho^{(1)}(\omega) + (n_A/2)\rho^{(2)}(\omega) \right], \tag{8}$$

$$n_B = 2\int_{-\infty}^{E_F} d\omega \left[(1-n_B/2)\rho^{(3)}(\omega) + (n_B/2)\rho^{(4)}(\omega) \right], \tag{9}$$

$$\rho^{(\nu)}(\omega) = -\frac{1}{\pi} \mathrm{Im} G^{(\nu)}(\omega). \tag{10}$$

From the self-consistent CPA equations (4) - (10) one can determine the local one-particle DOS $\rho_{A/B}(\omega)$, the occupation numbers n_A, n_B and the double occupancies d_A, d_B as functions of the model parameters Δ, U_A and U_B. A metal is distinguished from an insulator by a finite total DOS at the Fermi level $\rho(E_F) = x\rho_A(E_F) + (1-x)\rho_B(E_F)$.

III. RESULTS AND DISCUSSION

For numerical results the input parameters are the local on-site energies $\varepsilon_A = \Delta/2, \varepsilon_B = -\Delta/2$, the interaction strengths U_A, U_B and the band filling n. We focus on the half-filled case with $x = 0.5$ and $n = 1$. Through this work we set W as the unit of the energy. Figure 1 shows the local DOS for each type of sites $\rho_A(\omega)$ and $\rho_B(\omega)$ for $U_A = 1.25, \Delta = 1.5$ and four values of U_B. The general appearance of the DOS displays four structures. Two of these structures are mainly composed of A states (solid lines) and the other two of B states (dotted lines). For $U_B = 0.1$ and 4.0, corresponding to the band insulating and Mott insulating phases, the DOS show a gap around the Fermi level E_F. In contrast, the DOS at E_F for $U_B = 1.0$ and 2.0 are nonzero, which indicate a metallic phase. It should be noted that, despite U_A keeps a constant value, the $A-DOS$ evolves remarkably when U_B changes. Similar behaviors of the DOS were also found in the DMFT study of this system [4].

Figure 1 demonstrates that for fixed Δ and U_A two transitions from a band insulator via a metallic state to a Mott insulator are found with increasing U_B. To clarify the nature of these insulating states we calculate the occupation numbers $n_{\alpha\sigma}$ and double occupancies $d_\alpha = < n_{\alpha\uparrow} n_{\alpha\downarrow} >$ with α being A and B. These quantities are plotted in Fig.2 for $U_A = 1.25$ and $\Delta = 1.5$. For small U_B, only B sites are occupied and A sites are almost empty, correlation effects are weak in the occupied B band and d_B is large. The corresponding insulating state is clearly a band insulator. As U_B is increased, the double occupancy rapidly decreases for B sites. For larger U_B, both types of site are strongly correlated with almost zero double occupancies and $n_{A\sigma} \approx n_{B\sigma} \to 1/2$. Therefore, the insulating state is a Mott-Hubbard insulator.

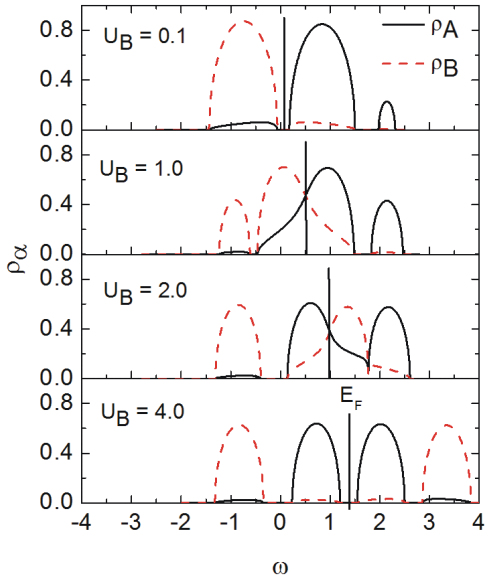

Fig. 1. Density of states for various values of U_B, for $U_A = 1.25$ and $\Delta = 1.5$ for the model at half-filling. Energy ω and parameters Δ, U_A, U_B are in energy unit set by $W = 1$. E_F refers to the position of Fermi energy.

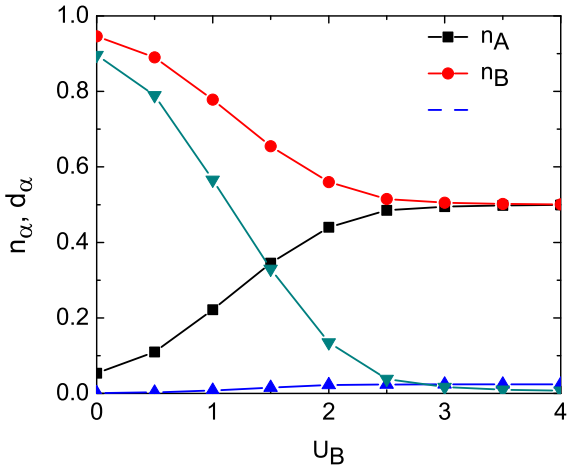

Fig. 2. Electronic occupation numbers and double occupancies as functions of U_B for $U_A = 1.25$ and $\Delta = 1.5$.

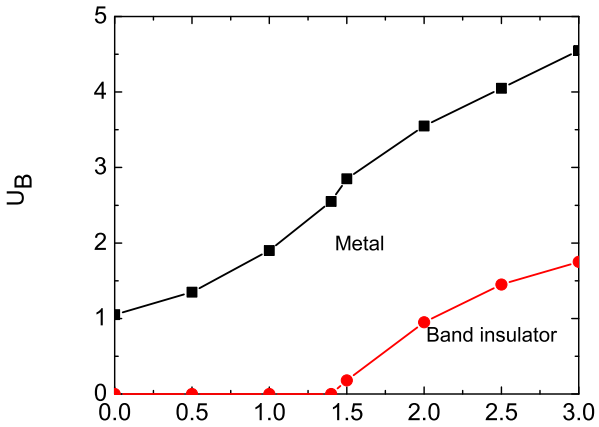

Fig. 3. Metal-insulator phase diagram at zero temperature for $U_A = 1.25$ for the fully diagonal disordered Hubbard model at half-filling.

Repeating the calculations for a fixed U_A and different values of Δ and U_B we constructed the metal-insulator phase diagram for the fully diagonal disordered Hubbard model at half-filling in the (Δ, U_B) plane, which we report in Fig.3. The shape of our metallic region is similar to those obtained in [4], keeping in mind that in our study the energy unit is the half-bandwidth W. It is interesting to note that paramagnetic solutions of the ionic Hubbard model at half-filling in dimensions $D > 2$ also indicate that the band and the Mott insulator phases are separated by a metallic phase [7-10].

IV. CONCLUSION

We have studied the MIT in the half-filled Hubbard model with full diagonal disorder by means of the coherent potential approximation. Within this approximation in combination with the semi-elliptical model for the bare DOS we calculate the site selective DOS, the corresponding occupation numbers and the double occupancies. For a fixed U_A, we derive the $U_B - \Delta$ phase diagram at zero temperature which is consistent with those obtained from DMFT by the NCA as the impurity solver at finite temperature.

The calculations presented here can be extended to the case away from half-filling and/or at finite temperature. Within the CPA one can also evaluate the temperature dependence of the conductivity and derive a phase diagram on the disorder-interaction plane. This is left to future work.

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